4,4'-Diaminostilbene 621-96-5 | DTXSID2022412

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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 27.1 days

Global applicability domain: Outside

Local applicability domain index: 2.64e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

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9-Ethyl-9H-fluorene Measured: 2330 Predicted: N/A Image not found

2-Methylphenanthrene Measured: 1370 Predicted: 25.0 Image not found

4-Phenyltoluene Measured: 4340 Predicted: 25.1

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1-Methyl phenanthrene Measured: 1370 Predicted: 36.9 Image not found

Benzothiophene Measured: 1650 Predicted: 21.4